ADVANCED COMPUTING FOR 21ST CENTURY ACCELERATOR SCIENCE & TECHONLOGY

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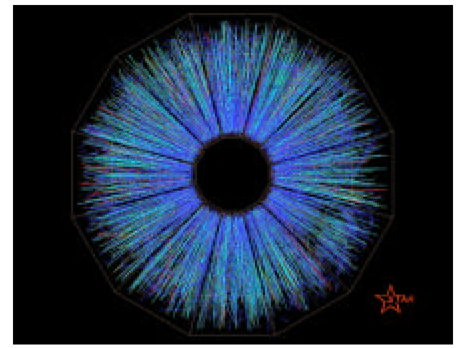
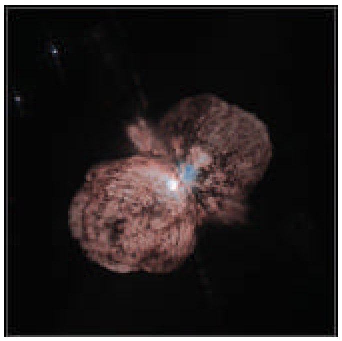
SciDAC PI Meeting – January 15-16, 2002

Accelerators Important to Office of Science

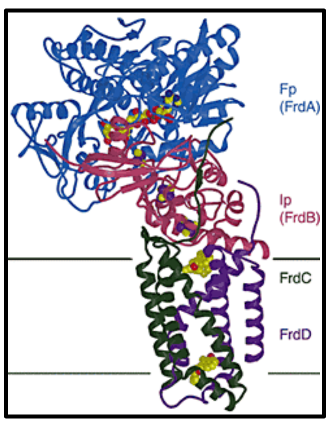
Accelerators are Crucial to Scientific Discoveries in High Energy Physics, Nuclear Physics, Materials Science, and Biological Science

"Starting this fall, a machine called RHIC will collide gold nuclei with such force that they will melt into their primordial building blocks"



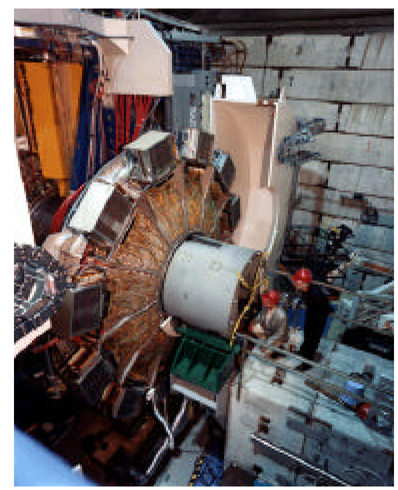


"A new generation of accelerators capable of generating beams of exotic radioactive nuclei aims to simulate the element-building process in stars and shed light on nuclear structure"

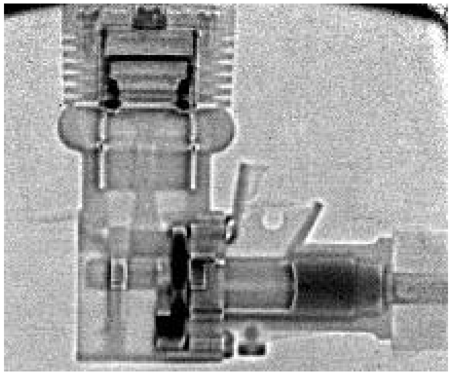


"Biologists and other researchers are lining up at synchrotrons to probe materials and molecules with hard x-rays"

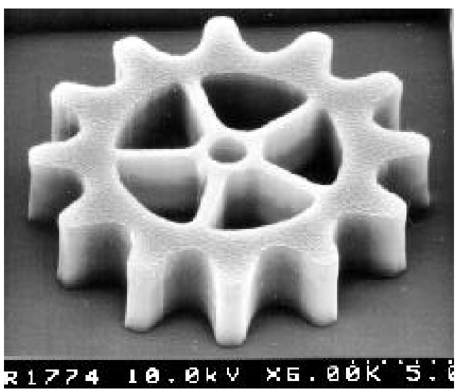
"Violated particles reveal quirks of antimatter"



Accelerators Beneficial to Society

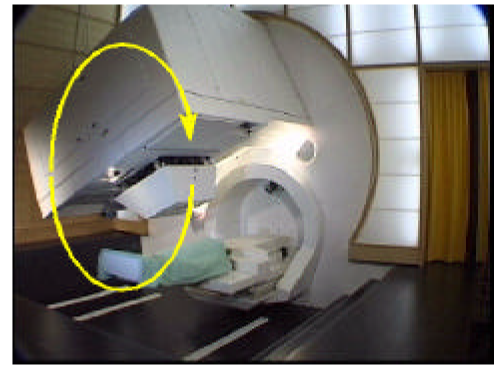


Proton Radiography for Industrial and National Security applications

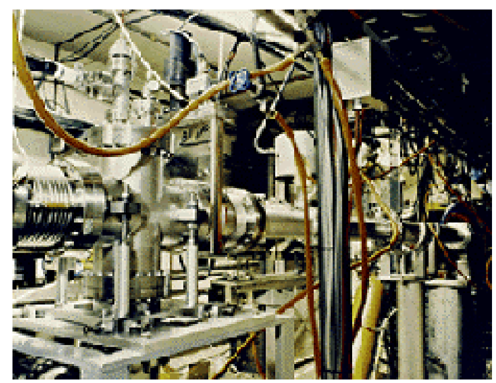


Beam Lithography

Medical Sterilization;
Food Irradiation;
Mail Irradiation



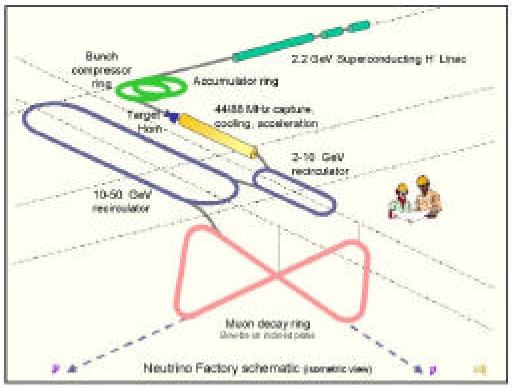
Medical Irradiation Therapy

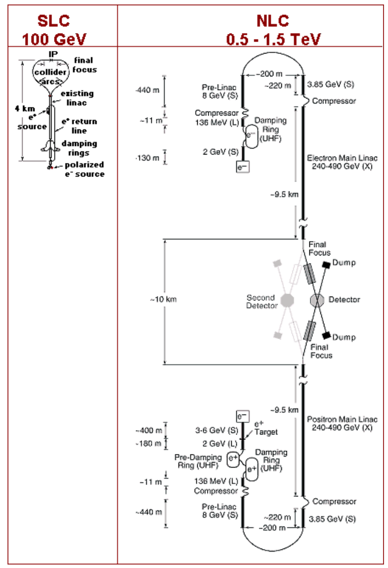


Medical Isotope Production

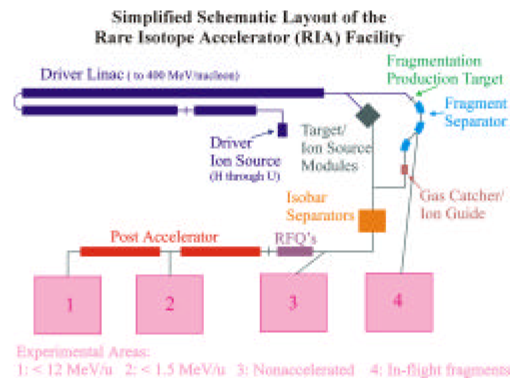
Opportunities at Next-Generation Accelerator Facilities

Exploring physics beyond the Standard Model. Are there new particles? New interactions?

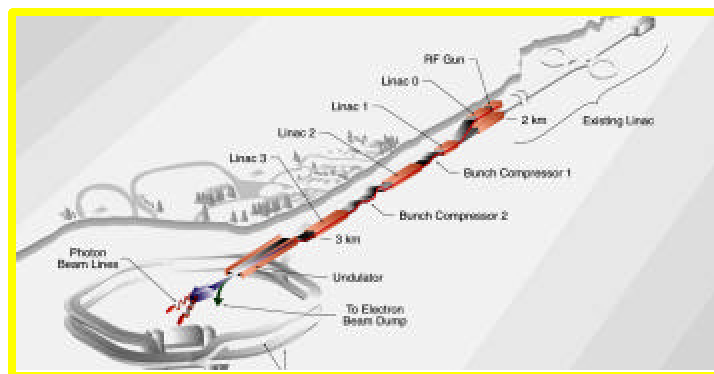




Research with exotic nuclei: The nature of nucleonic matter; origin of the elements; tests of the Standard Model



Research using intense, ultra-short pulses of x-ray radiation (4th generation light source): fundamental quantum mechanics; atomic, molecular, and optical physics; chemistry; materials science; biology



Accelerator Simulation Environment (ASE)

This project will develop a comprehensive terascale simulation capability, the **Accelerator Simulation Environment** (ASE), whose components will enable accelerator physicists and engineers to address a broad range of important issues in next-generation accelerators and their design. Using terascale resources and built on scalable algorithms, the software components and application codes in the ASE will be able to deliver the accuracy and resolution necessary for accelerator designs that are pushing the envelope of machine performance and system complexity.

The NEW set of parallel, portable, reusable, object-based software components will have an impact in three areas:

- **Designing next-generation accelerators** (NLC, a neutrino factory, RIA, a 4th generation light source, and a prototype fusion driver)
- **Optimizing existing accelerators** (PEP-II, RHIC, and the Tevatron)
- **Developing new accelerator technologies** such as laser- and plasma-based accelerators.

The ASE Team

- **National Labs:** LBNL – R. Ryne, J. Qiang, E. Esarey
  E. Ng (TOPS), C. Yang, P. Husbands
  SLAC – K. Ko, C. Ng, Z. Li, V. Ivanov, J. Tran, M. Wolf,
  N. Folwell, A. Guetz
  LANL – S. Habib, T. Mottershead, K. Campbell,
  C. Rasmussen (CCTTSS)
  FNAL – P. Spentzouris, F. Kamal, S. Uruppattu
  BNL – R. Samulyak
  SNL – P. Knupp (TSTT)

- **Universities:** Stanford – G. Golub, Y. Sun, W. Mi, I. Malik, Y. Muliadi
  UCLA – W. Mori, V. Decyk, C. Huang
  UCD – K. Ma, G. Schussman
  USC – T. Katsouleas, S. Deng
  U. Maryland – A. Dragt

- **Industry:** TechX – D. Bruhwiler

ASE - Target Applications

Development of the ASE will be guided by target applications that are computationally challenging, have maximum impact on HENP projects, and will serve as test-beds for the ASE.

- **Full-scale Modeling of Large Accelerating Structures**
  - > PEP-II interaction region to study beam heating
  - > entire NLC accelerator structure to calculate wakefields
  - > proposed radio frequency quadrupole (RFQ) design for RIA
- **Large-scale Beam Dynamics Simulations** for improving the performance of
  - > colliders (e.g. PEP-II, the Tevatron, and RHIC)
  - > high intensity drivers (the FNAL booster and BNL AGS)
- **Large-scale PIC Simulations** of
  - > plasma wakefield accelerators (particularly with regard to the critical issues of staging and emittance control),
  - > laser wakefield accelerators, including particle injection, capture, and acceleration

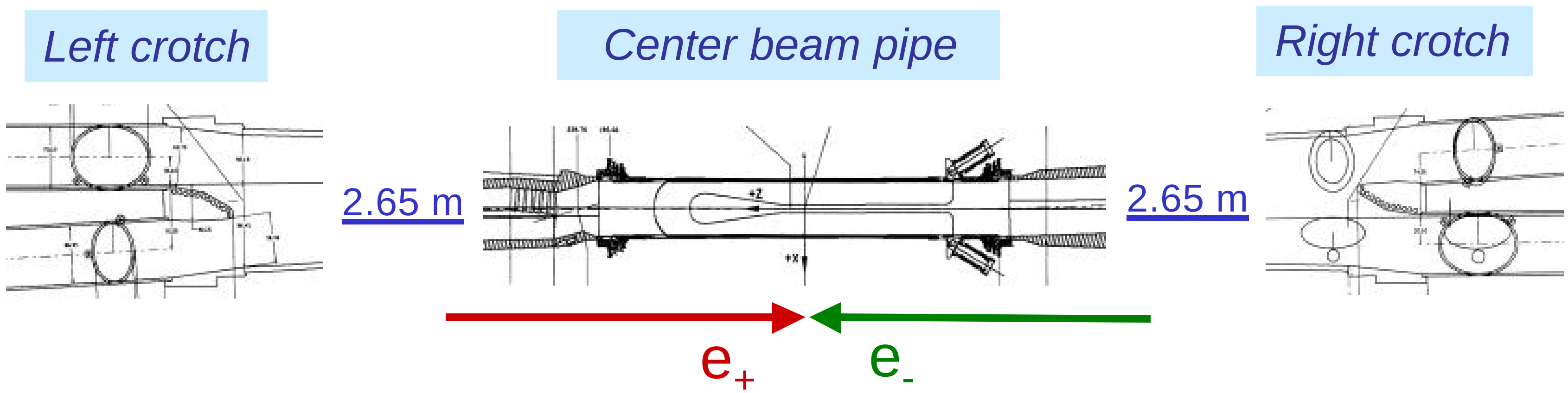
ASE - Deliverables

The ASE will concentrate on three areas:

- **Electromagnetics (EM)** – development of three 3D parallel field solvers that use unstructured grids to conform to complex geometries:
  - > Omega3P – Eigenmode code
  - > Tau3P – Time-Domain code
  - > Phi3P – Statics code
- **Beam Dynamics (BD)** – development of modules for treating multiple beam phenomena (such as space charge effects, high-order optical effects, beam-beam collisions, wakefields, intrabeam scattering, and ionization cooling), and their incorporation into a parallel version of the MaryLie/IMPACT beam dynamics code.
- **Advanced Accelerators (AA)** – development of the OSIRIS, VORPAL/XOOPIC and quickPIC codes for modeling laser- and plasma-based accelerators.

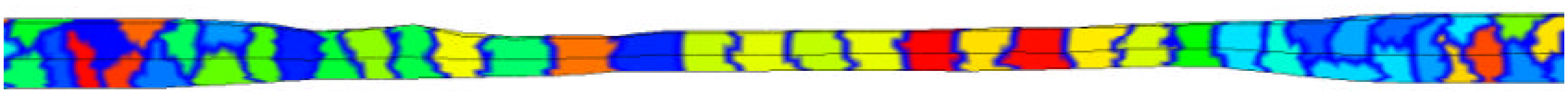
EM Work in Progress – PEP-II Interaction Region

Omega3P is used to study beam heating in the IR beamline complex

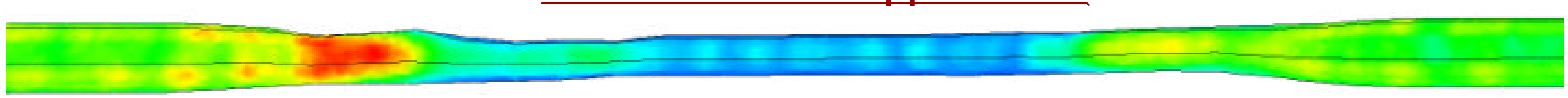


Mesh Model of a Section of the IR Beam Line centered around the Interaction Point

Domain Decomposition



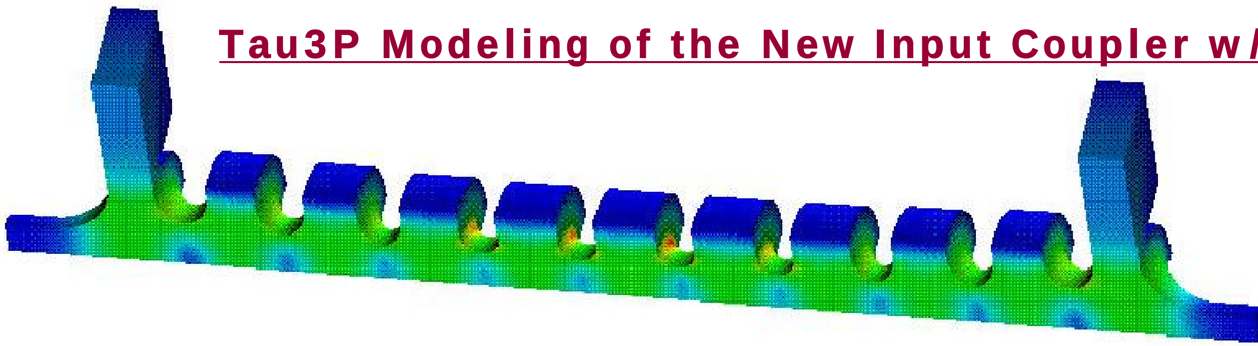
Wall Loss of a Trapped Mode



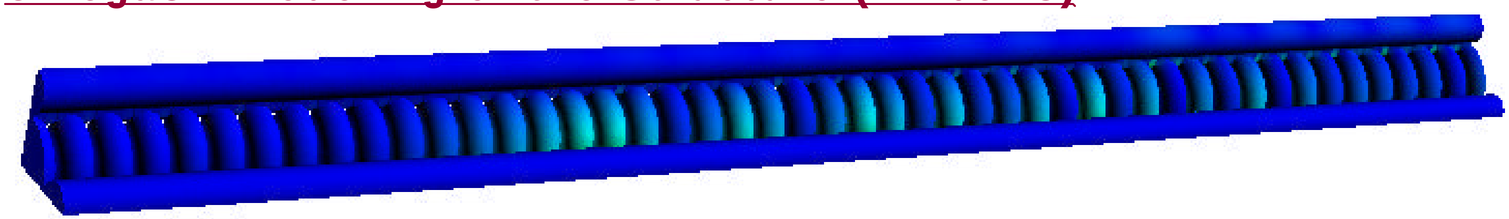
EM Work in Progress – NLC Structure Design

Omega3P and **Tau3P** are essential tools for the design of the **NEW** NLC accelerating structure which will have lower surface fields to avoid RF breakdown at high gradients. New structure has a lower group velocity and is shorter in length (< 100 cells).

Tau3P Modeling of the New Input Coupler w/ Inline Taper



Omega3P Modeling of the Structure (47 cells)



End to end simulation of the entire accelerating section is next

BD Work in Progress

- **Software Development and Applications**
  - MaryLie/IMPACT extended to use operator-splitting inside bending magnets (to model space charge in circular machines)
  - Wakefield module (resistive wake) developed and put into MaryLie
  - IMPACT used to model LEDA halo expt and novel SC linac designs
  - Effort underway to model FNAL booster with MaryLie/IMPACT
- **Model Evaluation and Code Benchmarking**
  - Systematic comparison of z-based vs t-based PIC codes
  - Analytical work on new exactly solvable models (incl. large-amplitude halo test problem) for code comparison and benchmarking
- **Algorithm Development**
  - Analysis of orthogonal method and development of new symplectic method to model infinite-dimensional Hamiltonian systems (e.g. wave equation, Maxwell's equations)
    - Orthogonal approach is unconditionally stable (no Courant condition)
    - Combines techniques from quantum dynamics, beam optics, FEM

AA Work in Progress

Code Development and Optimization

- OSIRIS
  - 2x single processor speed improvement
  - Begun to add ionization by adding particle creation module
- VORPAL/XOOPIC
  - Added parallel 3D field solver with fluid source terms
- quickPIC
  - Added parallel Poisson solver and particle push for conducting boundary
  - Developed framework for adding full quasi-static equations
  - Begun discussions with APDEC on adding parallel AMR

Production Runs

- OSIRIS: First full-scale 3D PIC simulations of Self-Modulated Laser Wakefield Acceleration. $2x10^8$ particles on 2000x152x152 mesh
- VORPAL/XOOPIC: Studied effects in LBL experiments using 2D PIC simulations with the new ionization package. Studied wakes using new 3D fluid code
- quickPIC: studied evolution of e^+ drive beam in E-162 expt at SLAC

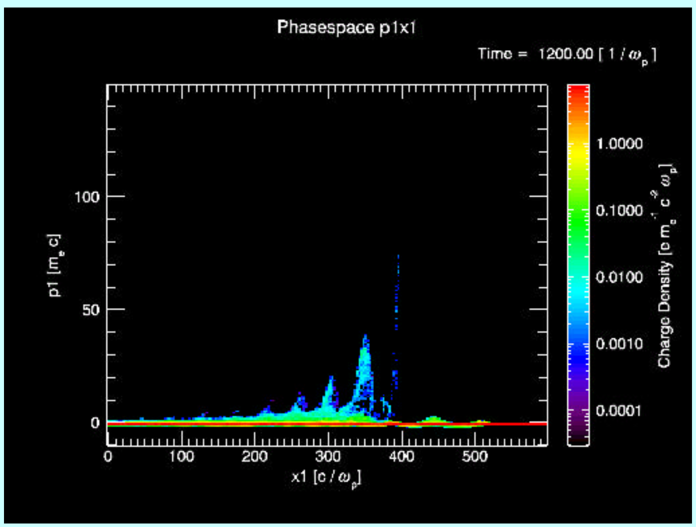
First 3D simulations of SMLWFA using OSIRIS : There are differences between 2D and 3D

3D simulations:
Laser: $a_o=3$, $t_{rise}=t_{fall}=116.5\omega_o^{-1}$ ($t_{fwhm}=35fs$), $w_o=38c/\omega_o$, $n/n_c=.02$
Physical dimension:$600c/\omega_o \times 300c/\omega_o \times 300c/\omega_o$
Grid size:2000x152x152 (4.6×10^7) with 4 particles/cell (2×10^8)
Run through 3 Rayleigh lengths (300um) and counting

200

γ

0

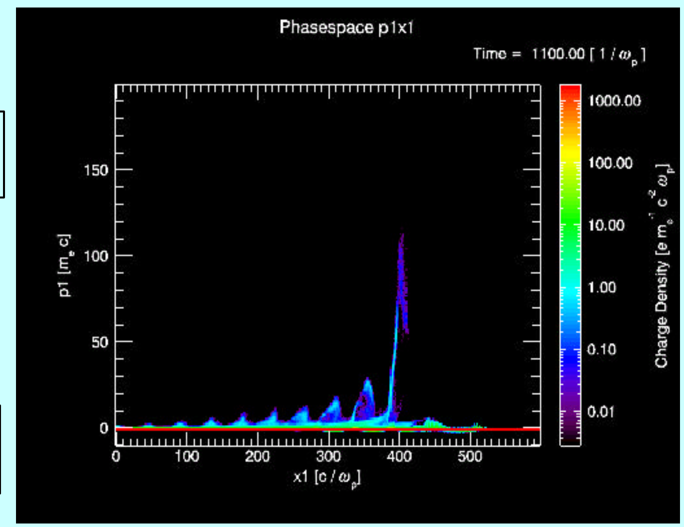


2D

200

γ

0



3D

Simulations are done at the SP2 at NERSC

ASE Partnerships in Applied Math & Comp. Sci.

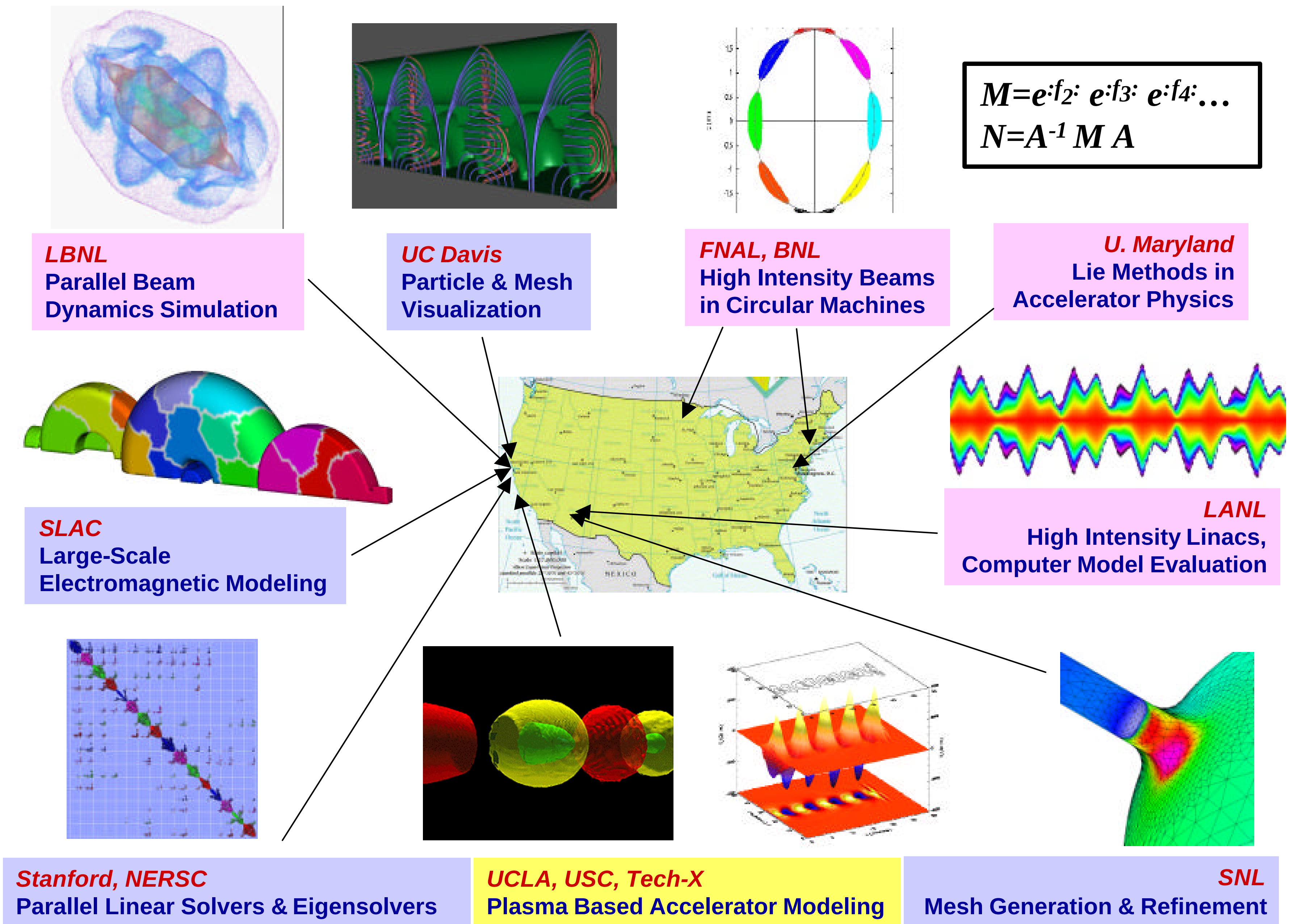
The success of the ASE will require close collaboration with applied mathematicians and computer scientists to enable the development of high-performance software components for terascale platforms.

Collaborating SciDAC Integrated Software Infrastructure Centers:

- **TOPS –** Eigensolvers, Linear Solvers
- **TSTT –** Mesh Generation & Adaptive Refinement
- **CCTTSS –** Code Components & Interoperability
- **APDEC –** Parallel Solvers on Adaptive Grids
- **PERC –** Load Balancing & Communication

Collaborating National Labs & Universities:

- **NERSC –** Eigensolvers, Linear Solvers
- **Stanford –** Linear Algebra, Numerical Algorithms
- **UCD –** Parallel Visualization, Multi-resolution techniques
- **LANL –** Statistical Methods for Computer Model Evaluation



$M=e^{:f_2:}\, e^{:f_3:}\, e^{:f_4:}\ldots$
$N=A^{-1}\, M\, A$
LBNL
Parallel Beam Dynamics Simulation
UC Davis
Particle & Mesh Visualization
FNAL, BNL
High Intensity Beams in Circular Machines
U. Maryland
Lie Methods in Accelerator Physics
SLAC
Large-Scale Electromagnetic Modeling
LANL
High Intensity Linacs, Computer Model Evaluation
Stanford, NERSC
Parallel Linear Solvers & Eigensolvers
UCLA, USC, Tech-X
Plasma Based Accelerator Modeling
SNL
Mesh Generation & Refinement

EM Collaboration with Stanford

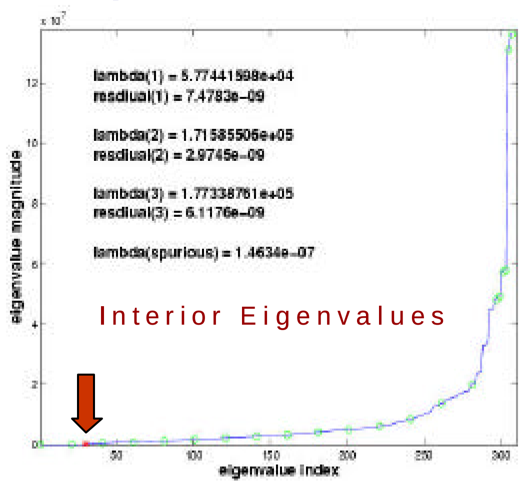
Omega3P solves the Matrix Eigenproblem: $\underline{K}\, x = l\, \underline{M}\, x$

- Inexact Shift-Invert Lanczos as Band Pass Filtering

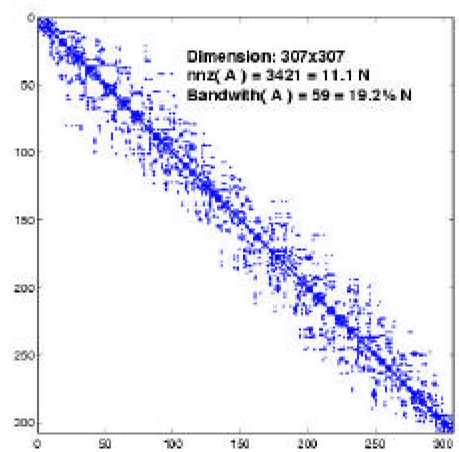
$$\frac{\left\| (\mathbf{K} - s\,\mathbf{I})\; v - q_i \right\|_2}{\left\| q_i \right\|_2} \leq e \quad \Rightarrow \quad \frac{\left\| d\,v \right\|_2}{\left\| v_0 \right\|_2} \leq e$$

- JOCC Refinement - Fixed Target, Real Arithmetic, No Search Space

Spectral Distribution

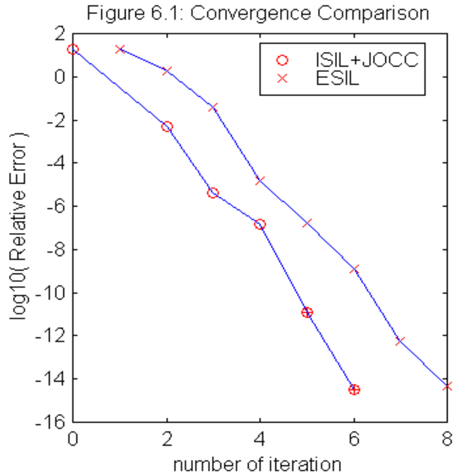


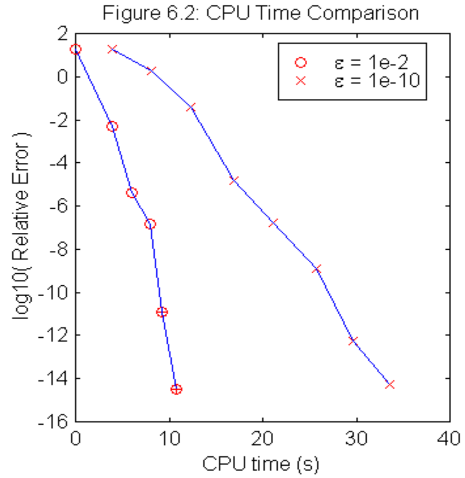
Matrix



EM Collaboration with NERSC/TOPS

Convergence





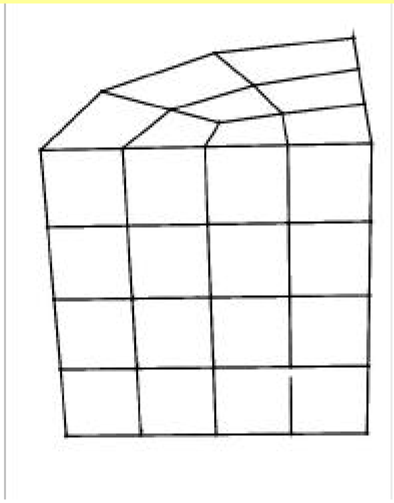
Omega3P – poor convergence in applications where the matrices are ill-conditioned and the eigenvalues are not well separated.

- NERSC/TOPS is implementing **MINRES** in place of GMRES for solving the JOCC linear system in the Jacobi iteration to improve convergence and reduce memory requirement.

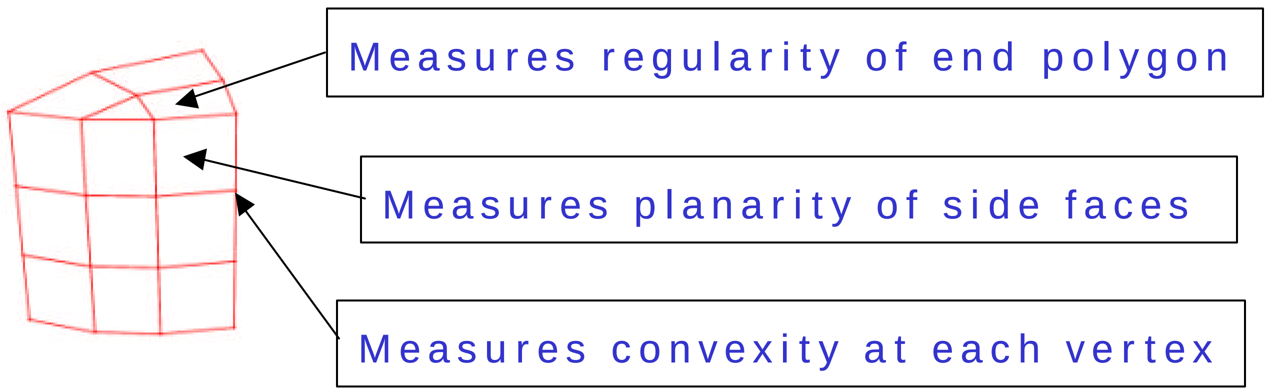
EM Collaboration with Sandia/TSTT

Tau3P – Parallel 3D Explicit Time-Domain Solver based on Dual, Staggered, Unstructured Grid. Good Mesh Quality is <u>essential</u> for Numerical Stability.

- Sandia/TSTT is developing **<u>Quality Metrics for Prismatic Elements</u>** which will enable the quality of primary and dual elements to be examined in swept hex meshes and how it effects the performance of Tau3p.



Primary Hex Mesh



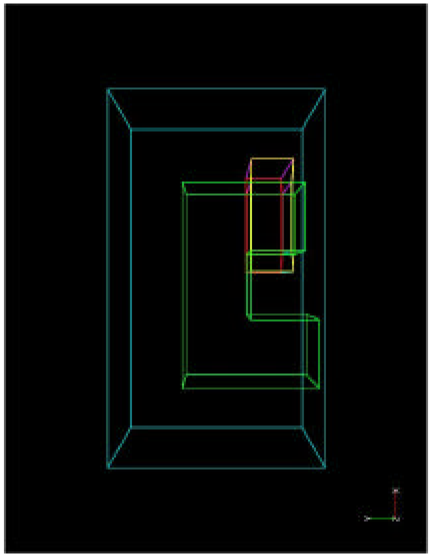
Corresponding Dual Mesh

EM Collaboration with Stanford

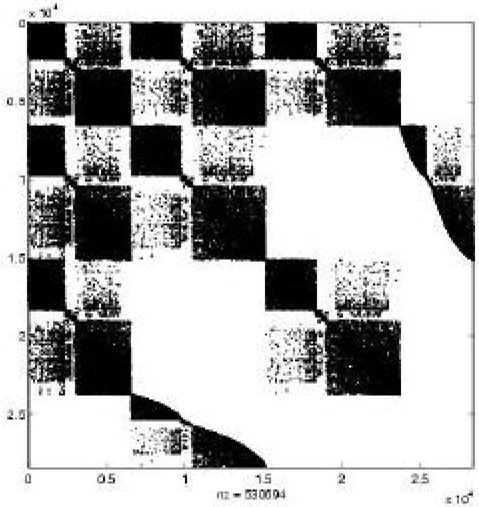
Phi3P – Parallel 3D Field-based Hybrid Finite Element Statics Solver for higher accuracy in fields & material boundary description

- Uses face element for B and edge element for H
- Large sparse symmetric indefinite structured matrix
- Existing libraries like Aztec fail for large systems
- New efficient and robust algorithms under development

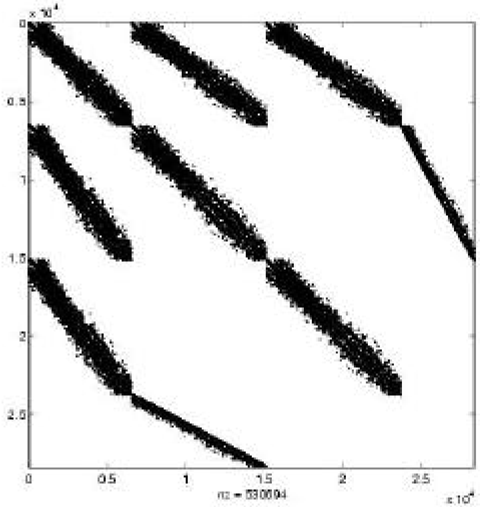
Sample Problem of a C Magnet



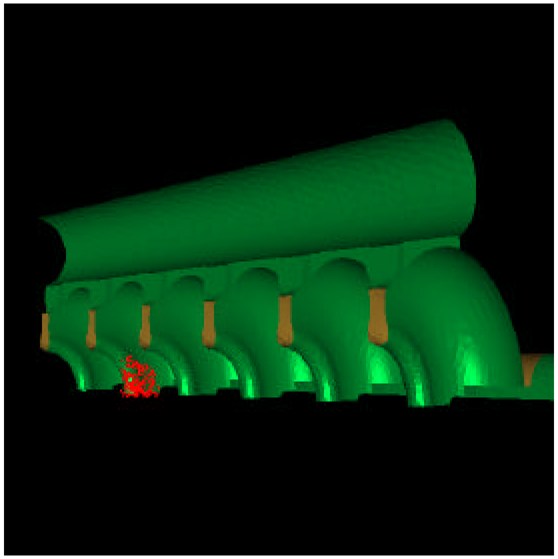
Matrix Pattern



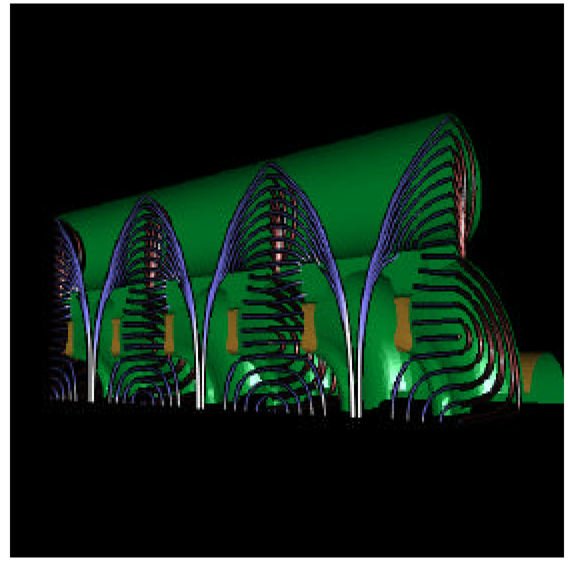
Matrix Pattern after Reordering



EM Collaboration with UCD



Particles



Electromagnetic Fields

- UCD is developing **Parallel Visualization Tools** for handling Large time-varying datasets on unstructured meshes that contain multiple complex vectors and particle motion

Advanced illumination and interactive methods will be used for displaying particles and fields simultaneously to locate regions of interest, and multi-resolution techniques will be deployed to overcome performance bottlenecks.

Summary

- Accelerators
  - -are enablers of great science
  - -advance technologies that are highly beneficial to the nation's health, wealth, and security

- Advanced computing, used in concert with experiment and theory, will enable new discoveries in accelerator science and technology

- SciDAC provides an excellent opportunity as well as the resources for HENP accelerator scientists and MICS researchers to foster a close collaboration in developing a terascale simulation capability for the accelerator community, the Accelerator Simulation Environment (ASE). The collaboration is now well underway.

- New tools and capabilities under development for the ASE are already having an impact on present accelerators and on the design of next-generation facilities.